Journal of Magnetism and Magnetic Materials 310 (2007) 1331–1333

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Enhanced low-temperature entropy and flat-band ferromagnetism in the $t - J$ model on the sawtooth lattice

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Received 7 June 2006

Abstract

Using the example of the sawtooth chain, we argue that the $t-J$ model shares important features with the Hubbard model on highly frustrated lattices. The lowest single-fermion band is completely flat (for a specific choice of the hopping parameters $t_{i,j}$ in the case of the sawtooth chain), giving rise to single-particle excitations which can be localized in real space. These localized excitations do not interact for sufficient spatial separations such that exact many-electron states can also be constructed. Furthermore, all these excitations acquire zero energy for a suitable choice of the chemical potential μ. This leads to: (i) a jump in the particle density at zero temperature, (ii) a finite zero-temperature entropy, (iii) a ferromagnetic ground state with a charge gap when the flat band is fully occupied and (iv) unusually large temperature variations when μ is varied adiabatically at finite temperature.

PACS: 71.10.Fd; 65.40.Gr

Keywords: flat band; localized states; frustrated lattice; $t-J$ model; entropy

During the past years, it has been noted that exact ground states can be constructed for the antiferromagnetic XXZ model at high fields on a large class of highly frustrated lattices (see [1,2,3] and references therein). This leads to a finite zero-temperature entropy exactly at the saturation field and an enhanced magnetocaloric effect [2,4,5,6], suggesting potential applications for efficient low-temperature magnetic refrigeration [4,7]. Recently, we have pointed out [8] analogies to flat-band ferromagnetism in the Hubbard model on the same lattices (see e.g. [9,10,11,12,13]).

Here we will illustrate some of the issues with exact diagonalization results for the $t-J$ model. The $t-J$ model arises as the large-U limit of the Hubbard model and is defined by the Hamiltonian

$$H = \sum_{\sigma} \sum_{\langle i,j \rangle} t_{i,j}\, P \left(c^{\dagger}_{i,\sigma} c_{j,\sigma} + c^{\dagger}_{j,\sigma} c_{i,\sigma} \right) P + \sum_{\langle i,j \rangle} J_{i,j} \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \frac{1}{4}\, n_i\, n_j \right) + \mu \sum_{i=1}^{N} n_i\,. \quad (1)$$

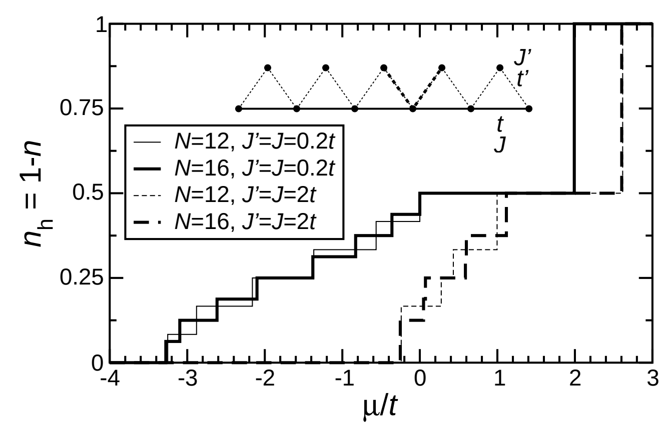

Fig. 1. Inset: The sawtooth chain model. Filled circles show electron sites. The hopping (magnetic exchange) are t (J) along the base line and t' (J') along the dashed zigzag-line, respectively. The bold valley shows the area occupied by a localized excitation. Main panel: Hole density $n_{\mathrm{h}} = 1 - n$ at temperature $T = 0$ as a function of chemical potential μ for $t' = \sqrt{2}\,t > 0$ and two choices of $J' = J$.

The sums run over the nearest-neighbor pairs $\langle i, j \rangle$ of a lattice with N sites. $c^{\dagger}_{i,\sigma}$ and $c_{i,\sigma}$ are the usual fermion creation and annihilation operators, P is the projector which eliminates doubly occupied sites, $n_i = c^{\dagger}_{i,\uparrow} c_{i,\uparrow} + c^{\dagger}_{i,\downarrow} c_{i,\downarrow}$ is the total number operator at site i, and $\boldsymbol{S}_i$ are spin-1/2 operators acting on an occupied site i.

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[1] Participation at ICM2006 supported by the DFG through SFB 602.

Here we will concentrate on the sawtooth chain model sketched in the inset of Fig. 1. The lower of the two branches of the single-electron dispersion becomes completely flat for $t' = \sqrt{2}\,t$. For this choice one can construct first localized single-electron excitations living in one of the valleys of the sawtooth chain (bold dashed line in the inset of Fig. 1), and then excitations with $N_{\rm el}$ electrons which are non-interacting for sufficient spatial separations and thus have energy $E = (-2\,t + \mu)\,N_{\rm el}$, in exactly the same manner as for the Hubbard model [8]. So far, the magnetic exchanges $J_{i,j}$ are arbitrary. However, it will turn out that they should be chosen sufficiently weak in order to ensure that the non-interacting localized many-electron states are the ground states in their respective particle number subspaces. At half filling $n = \langle n_i \rangle = 1$ only the magnetic part of the $t-J$ model survives such that it reduces to the previously studied antiferromagnetic spin-1/2 Heisenberg model (see [1,3,4,5,6] for the sawtooth chain).

The main panel of Fig. 1 shows finite-system results for $n_{\rm h} = 1-n$ at $T = 0$ versus μ for $t' = \sqrt{2}\,t$ (these curves are the electronic counterpart of the magnetization curves [3]). For small magnetic exchange (like $J' = J = 0.2\,t$), there is a jump of height $\delta n = 1/2$ exactly at $\mu = 2\,t$. At this point, all localized many-electron excitations collapse to $E = 0$. Furthermore, for $N = 12$ the number of ground states is 1, 12, 54, 112, 105, 36, 7 in the sectors with $N_{\rm el} = 0$, 1, 2, 3, 4, 5, 6, respectively. This leads to a ground-state entropy per site $\ln(327)/12 = 0.48\ldots$ at $\mu = 2\,t$ for $N = 12$. The ground-state degeneracies are exactly the same as for the Hubbard model [14] consistent with the ground states of the $t-J$ model for small $J_{i,j}$ and $N_{\rm el} \leq N/2$ being projections of those of the Hubbard model. General theorems for the Hubbard model imply a saturated ferromagnetic ground state for $N_{\rm el} = N/2$ (see e.g. [11,12,13] for the sawtooth chain). Numerically, we find a fully saturated ferromagnet for the $t-J$ model in the sectors with $N_{\rm el} = N/2$ and $N/2-1$. The plateau at $n = N_{\rm el}/N = 1/2$ in the $n(\mu)$-curve in Fig. 1 shows that the ground state is a saturated ferromagnet for $0 < \mu < 2\,t$, corresponding to an appreciable charge gap.

The situation changes for larger antiferromagnetic $J_{i,j}$, as illustrated for $J' = J = 2\,t$ in Fig. 1. In this case the localized states are no longer the lowest-energy states. This is signalled by a shift of the jump between $n = 1/2$ and $n = 0$ to $\mu > 2\,t$ which now corresponds to a true first-order transition. The charge gap, *i.e.*, the plateau at $n = 1/2$ is also present in this case.

The ground-state degeneracies are reflected by thermodynamic properties, as illustrated for the entropy S in Fig. 2 (the curves of constant S correspond to the adiabatic demagnetization curves of the magnetic counterpart [4]). In particular, the finite $T = 0$ entropy at $\mu = 2\,t$ leads to large temperature changes during adiabatic variations of μ, even cooling to $T = 0$ as $\mu \to 2\,t$ at low temperatures. The low-temperature properties for μ close to $2\,t$ are controlled by the localized states and are independent of the details of the microscopic model ($J_{i,j}$ in the $t-J$ model and U in

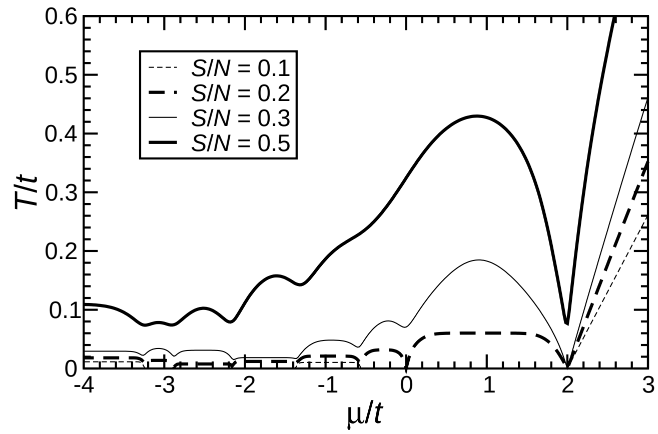

Fig. 2. Curves of constant entropy S for $t' = \sqrt{2}\,t > 0$, $J' = J = 0.2\,t$, and $N = 12$ sites.

the Hubbard model [14]); finite-size effects are also small in this region. By contrast, the behavior for $\mu < 0$ in Fig. 2 exhibits strong finite-size effects at low temperatures and depends on details of the model: for example, in this region the presence of doubly occupied sites leads to qualitatively different behavior of the Hubbard model [14].

We have focussed on the sawtooth chain, but it should share important features with a large class of highly frustrated lattices such as the kagomé lattice [1,6,9] which do not require any fine-tuning. We expect that the $t-J$ model with weak $J_{i,j}$ has the same localized excitations as the repulsive Hubbard model such that it shares in particular the same properties with respect to flat-band ferromagnetism [9,10,11,12,13]. The main advantage of the $t-J$ model is a substantially reduced Hilbert space dimension close to $n = 1$ which simplifies a full diagonalization and thus the exact determination of finite-temperature properties of a finite system.

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